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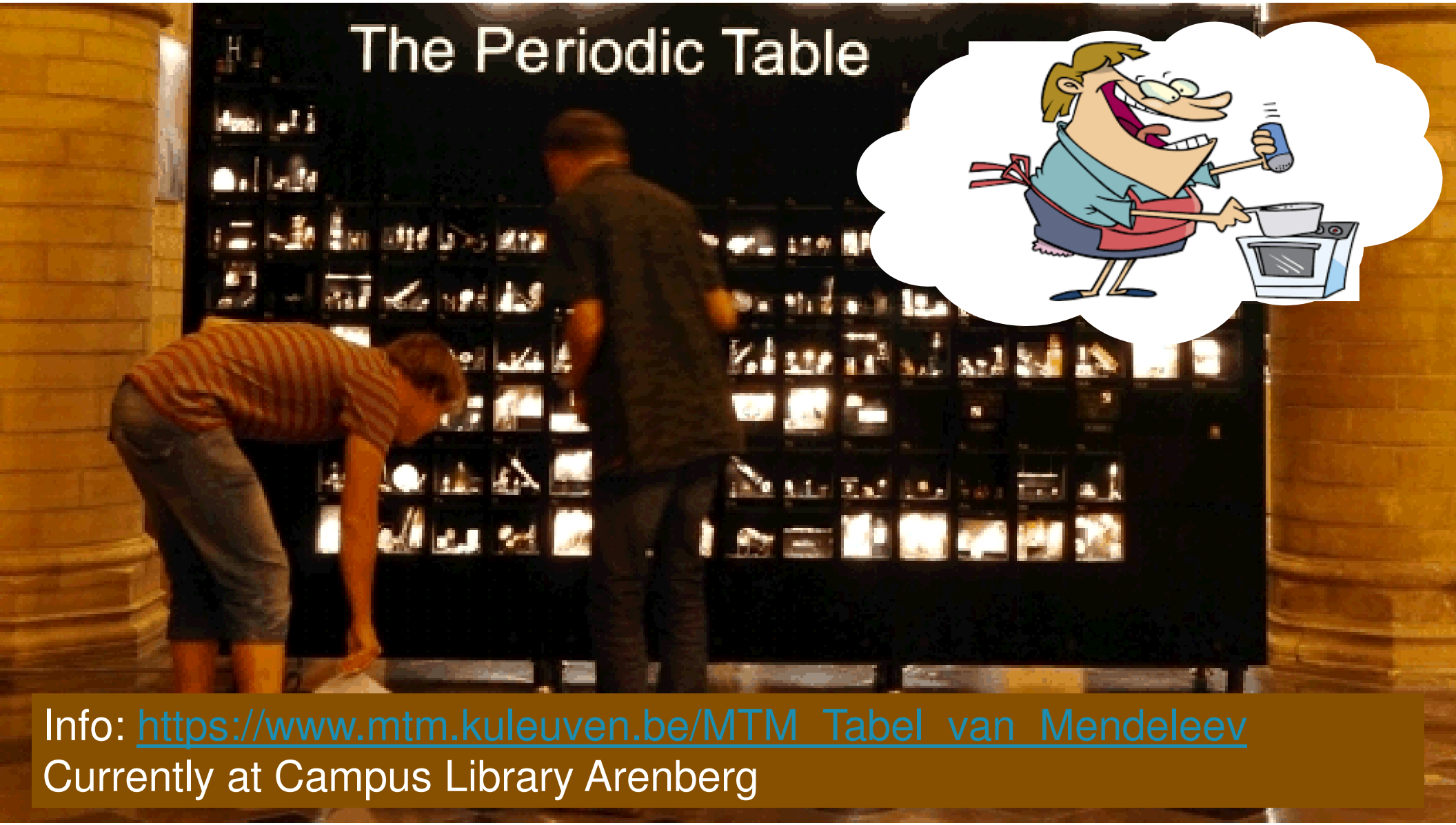
European Research Council

Unraveling interdiffusion effects at material interfaces – Learning from tensors and large-scale computer simulations

Nele Moelans

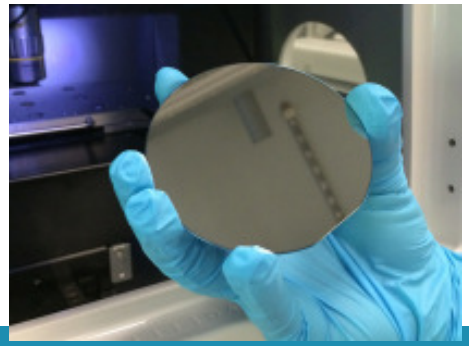
March 9, 2017

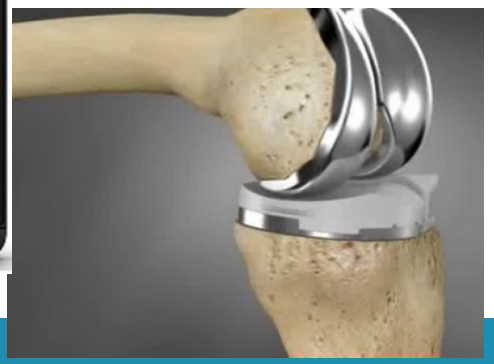


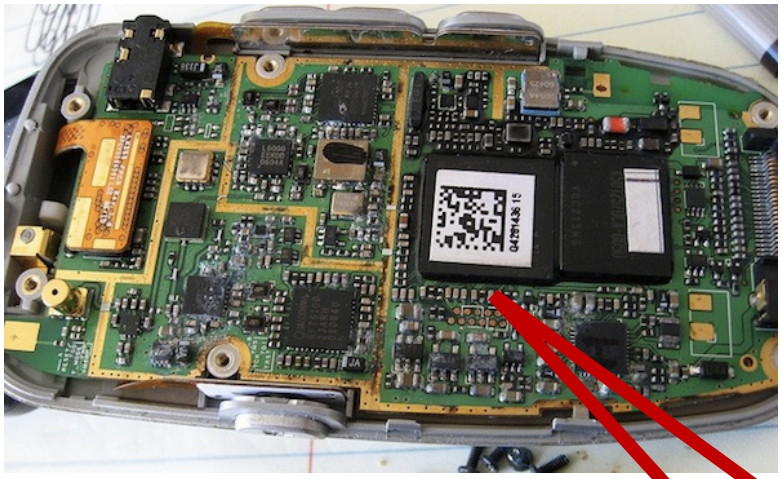
Info: https://www.mtm.kuleuven.be/MTM_Tabel_van_Mendeleev
Currently at Campus Library Arenberg

More principle elements in new materials

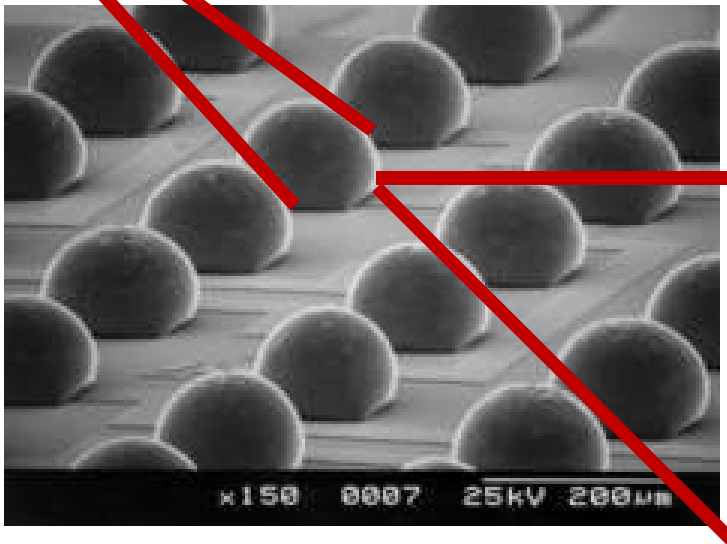
- Super alloys
- Magnetic materials
- New solar cell materials
- High-entropy alloys
- …

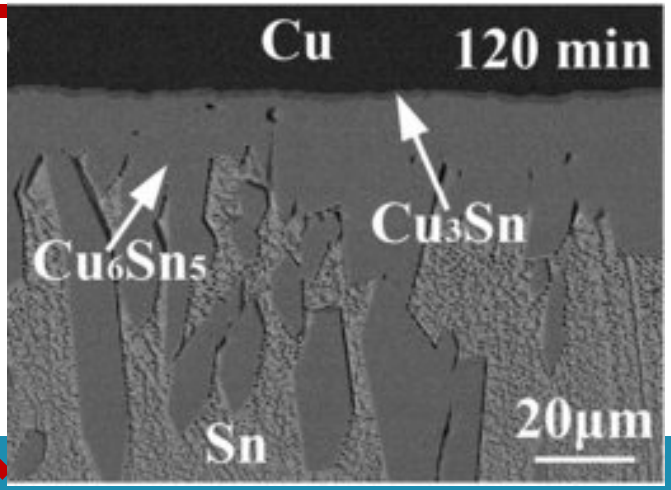


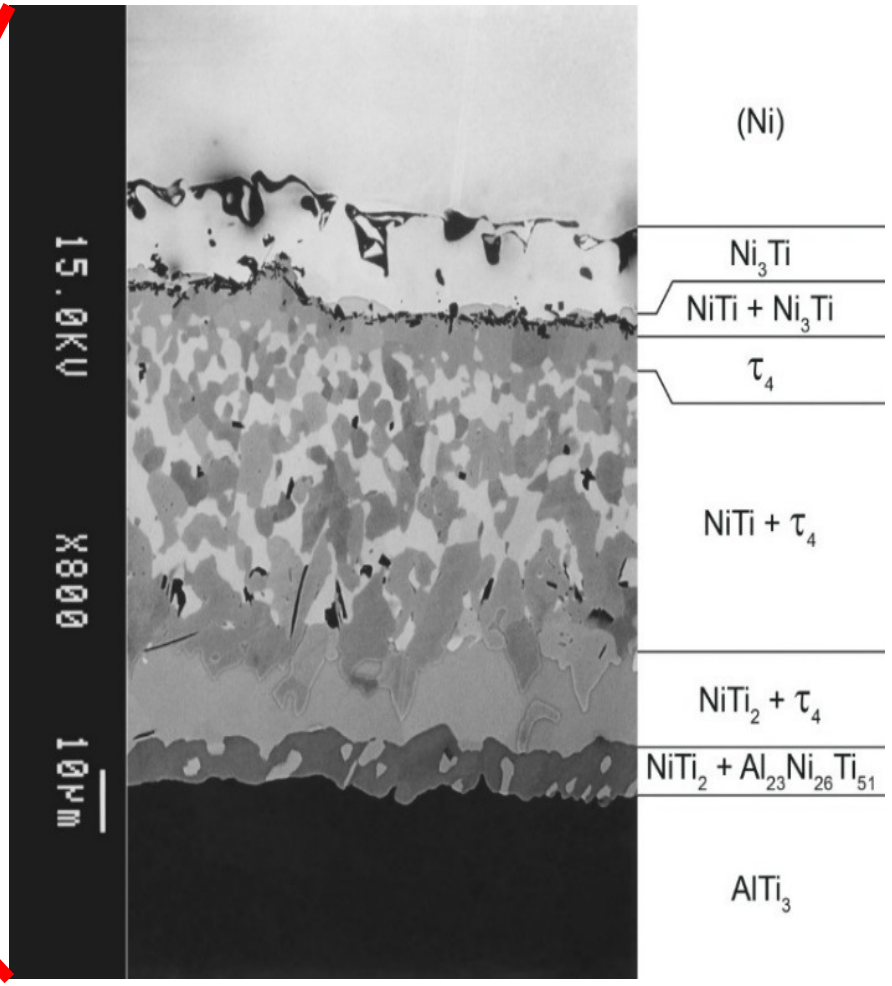




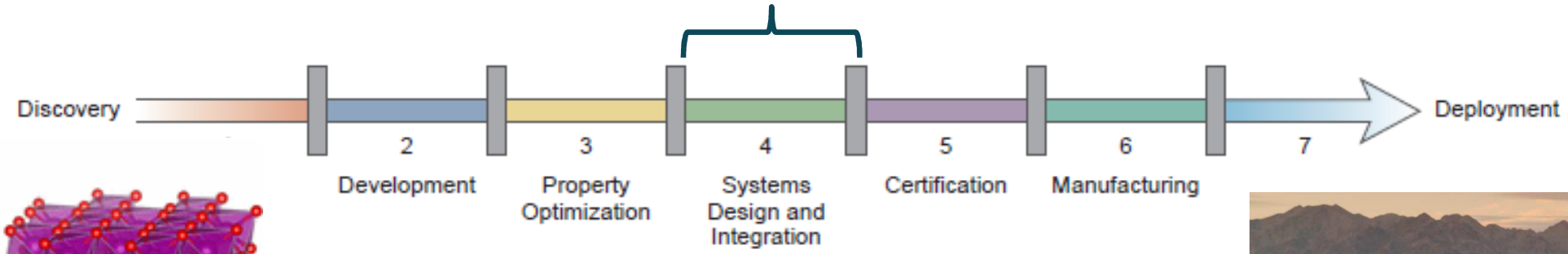

BlackBerry Hub
BlackBerry

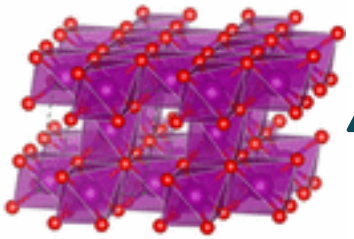

x150 0007 25kV 200µm


Cu
120 min
Cu6Sn5
Cu3Sn
Sn
20µm

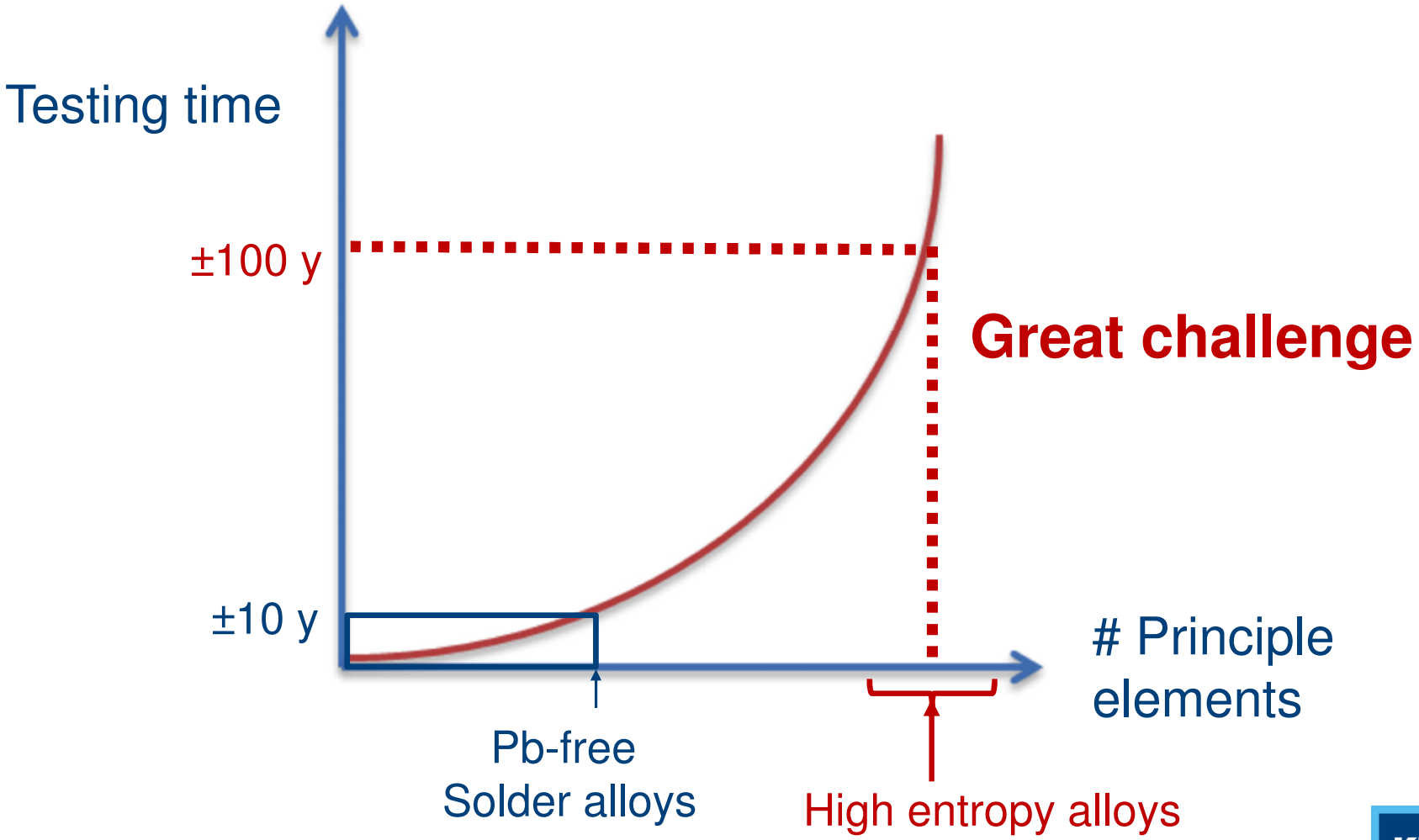

15.0KV X800 10μm
(Ni)
Ni_3Ti
$NiTi + Ni_3Ti$
τ_4
$NiTi + \tau_4$
$NiTi_2 + \tau_4$
$NiTi_2 + Al_{23}Ni_{26}Ti_{51}$
$AlTi_3$

Long testing times
high degree of trial-and-error

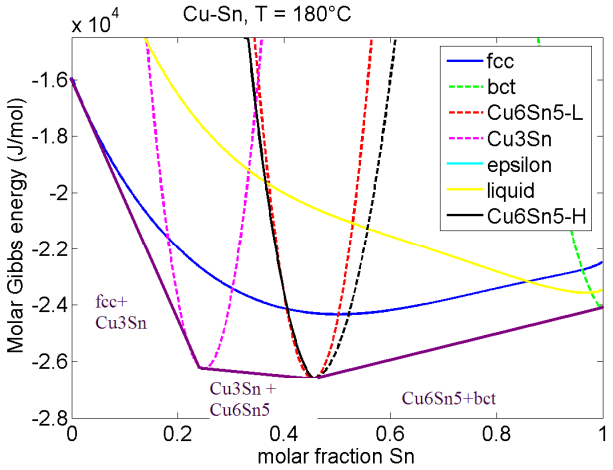




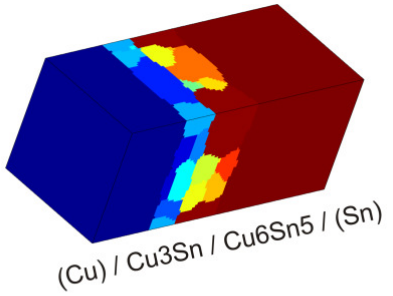
Numerous iterations

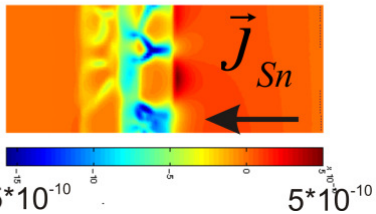

Testing time
±100 y
±10 y
Great challenge
Principle elements
Pb-free Solder alloys
High entropy alloys

Thermodynamic models/databases

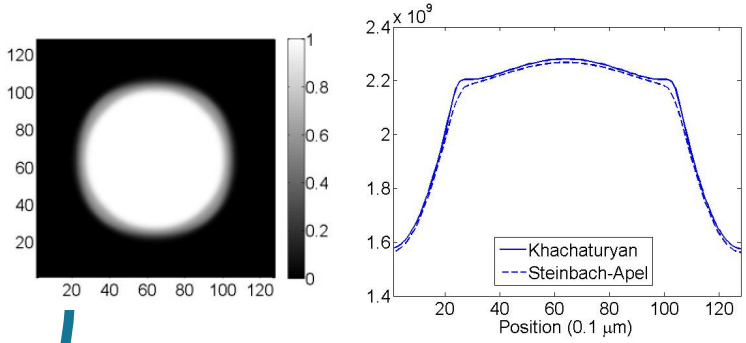


Phase field simulations

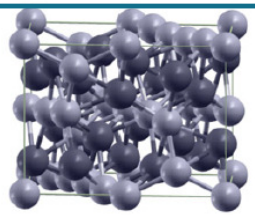




Mechanical models

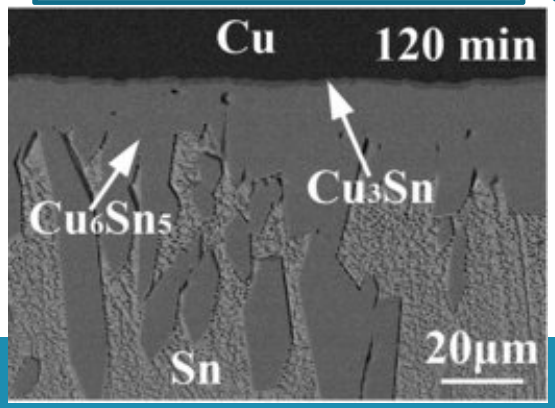


Atomistic models

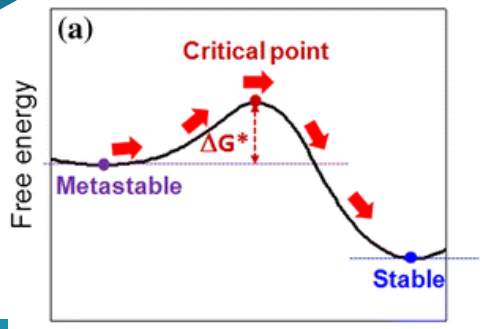


η'-cu6sn5

Experiments



Nucleation theory



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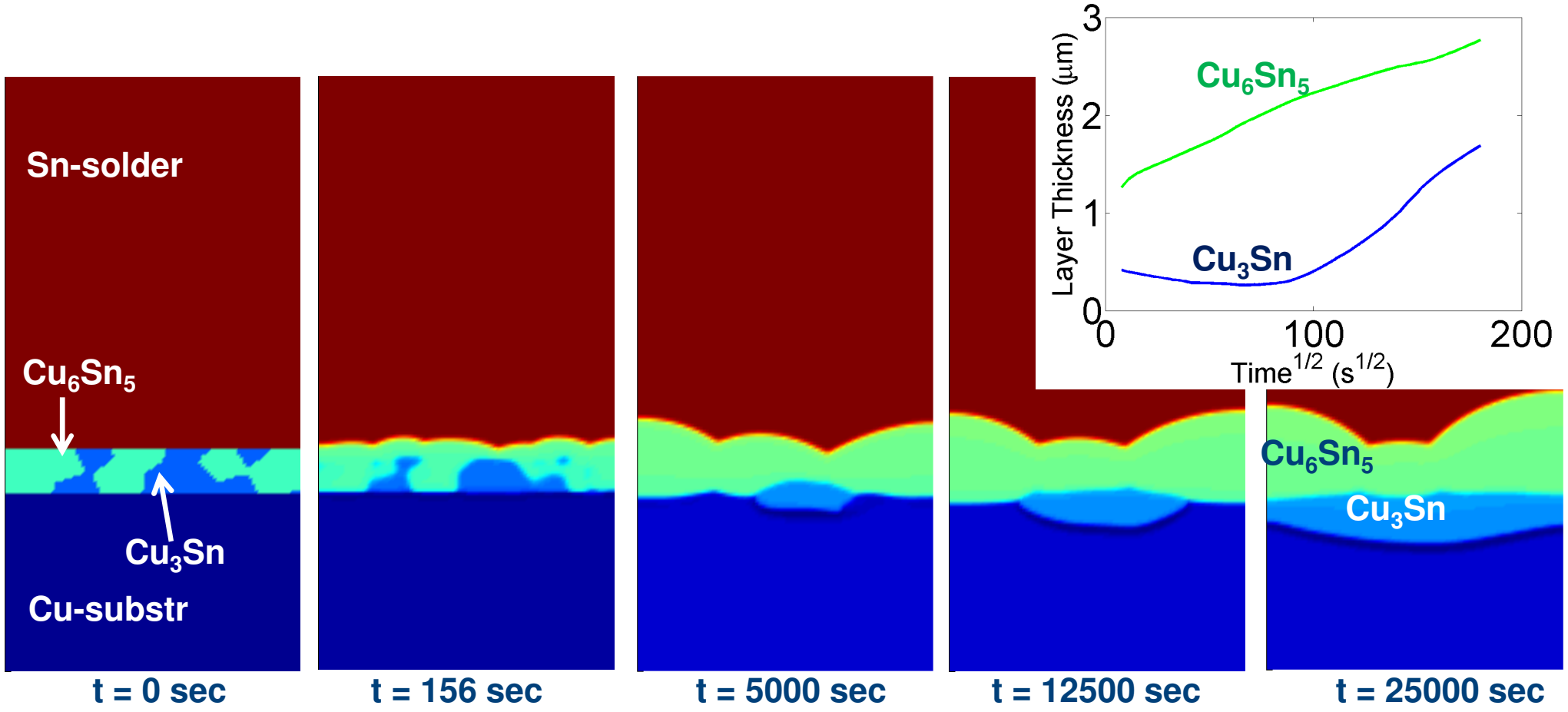
Sn-solder
Cu6Sn5
Cu3Sn
Cu-substr
t = 0 sec
t = 156 sec
t = 5000 sec
t = 12500 sec
t = 25000 sec
Layer Thickness (μm)
Time1/2 (s1/2)
Cu6Sn5
Cu3Sn
0
1
2
3
0
100
200

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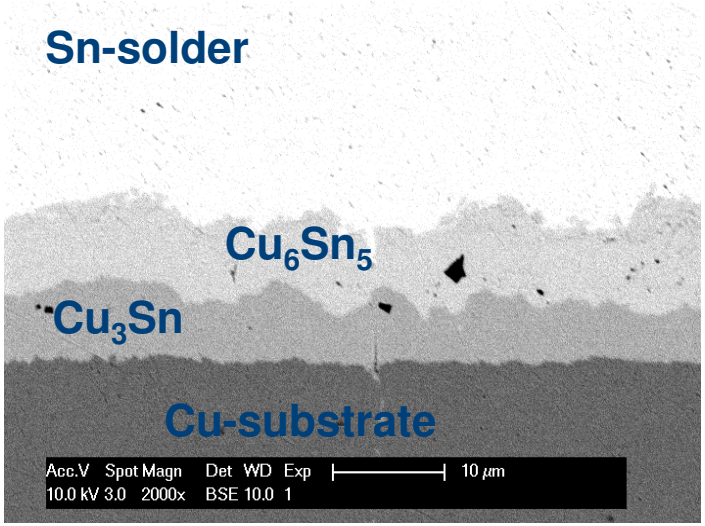
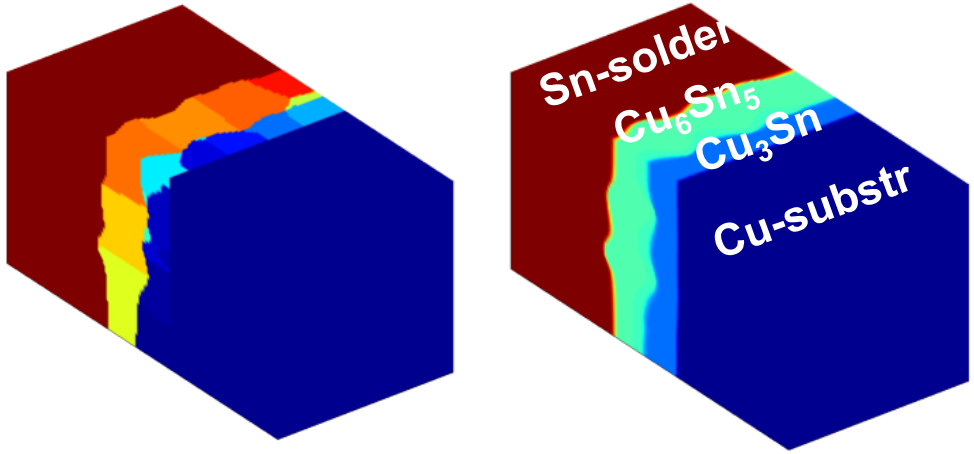


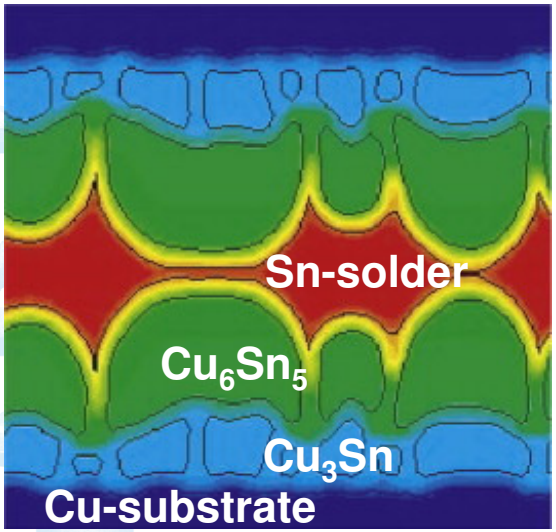


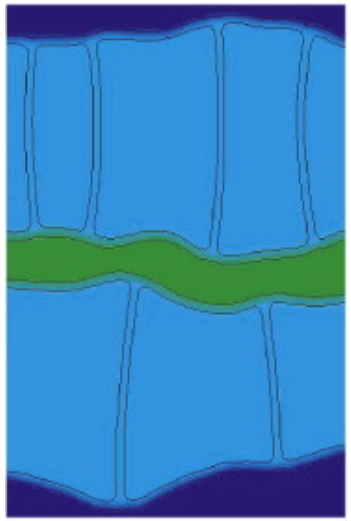
Solid state bonding at 170 °C, 840 h

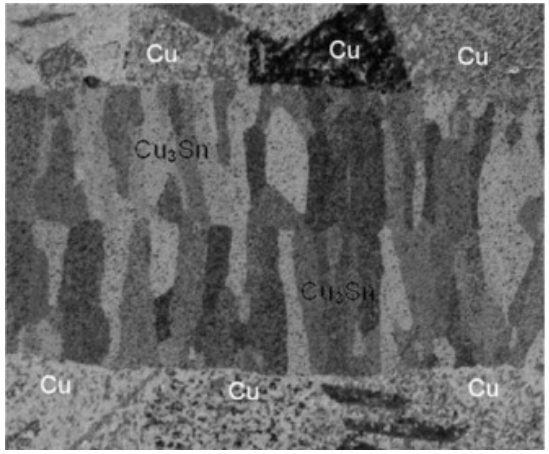
NM9

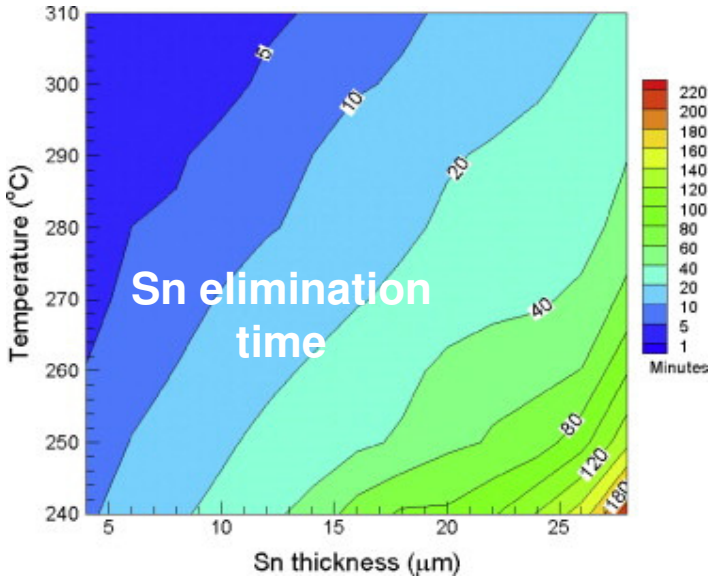
Transient Liquid Phase bonding

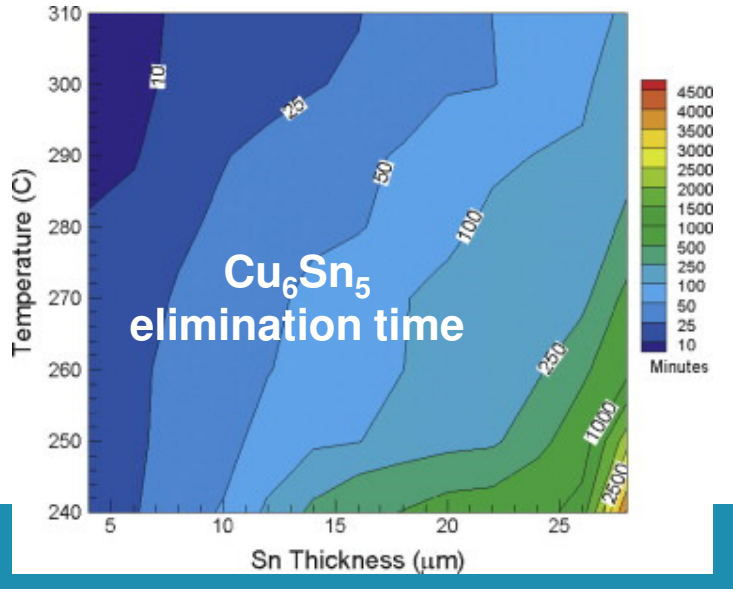
Cu / Sn-solder / Cu sandwich structure









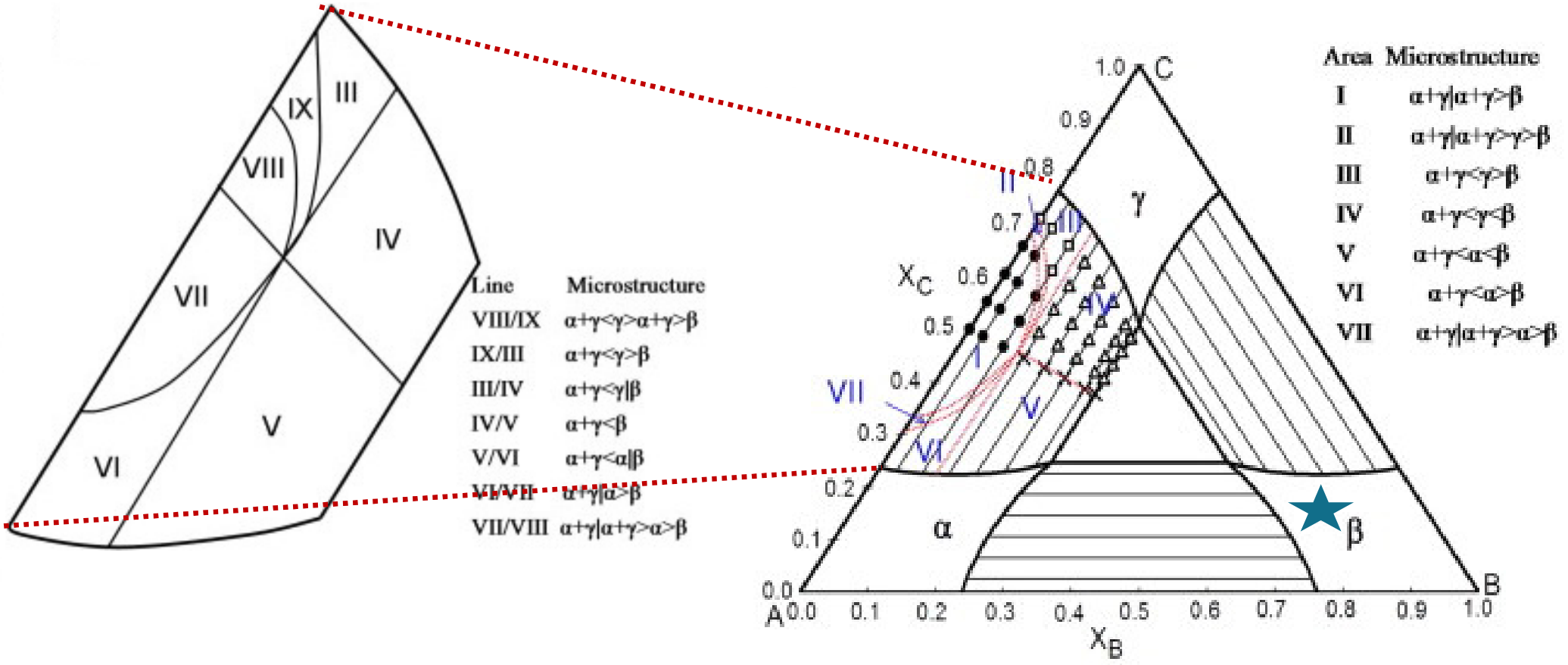


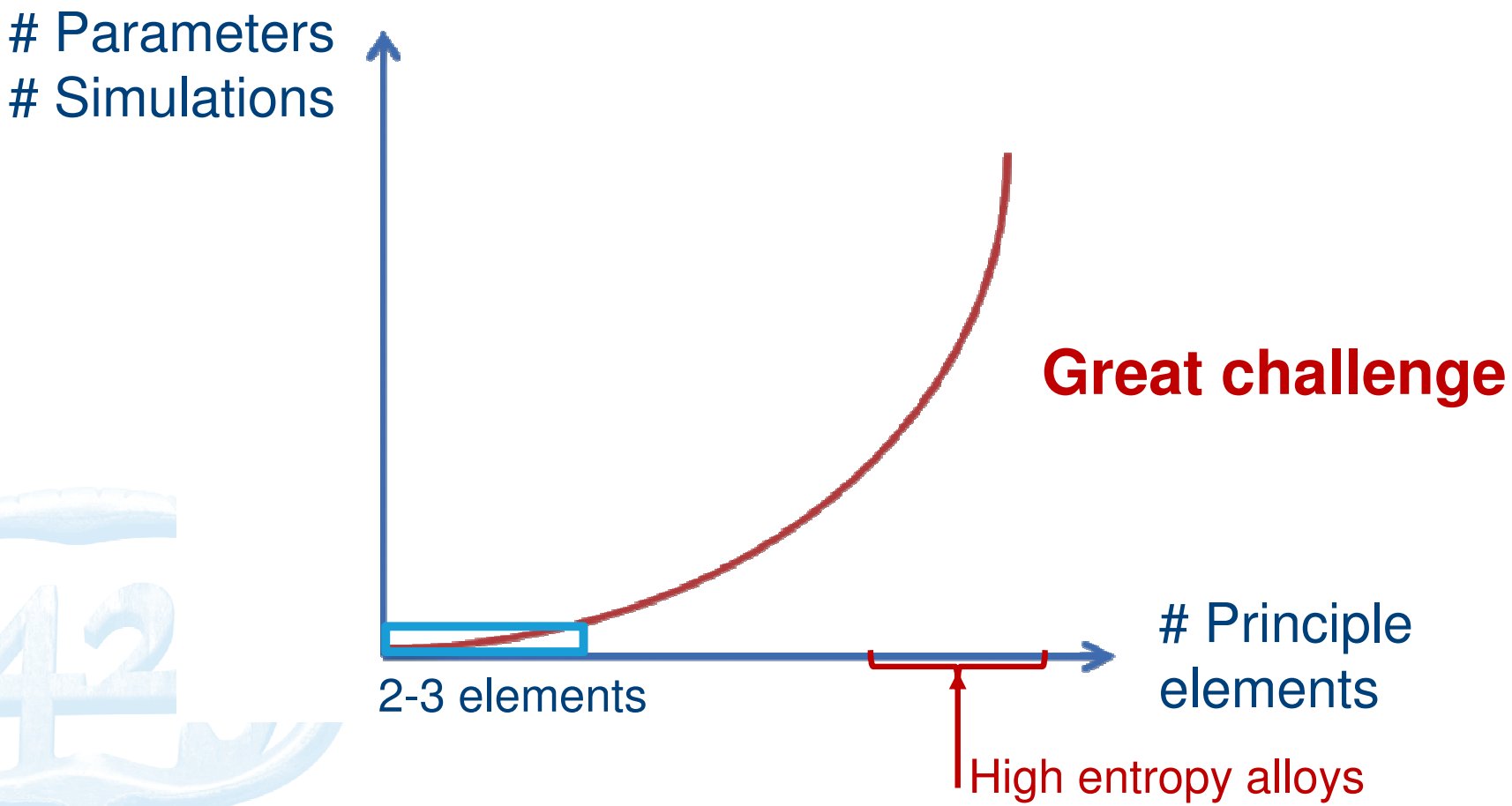
M.S. Park, S.L. Gibbons, R. Arróyave, Acta Materialia, 60, 2012, 6278–6287.

Slide 11

NM9 reference toevoegen

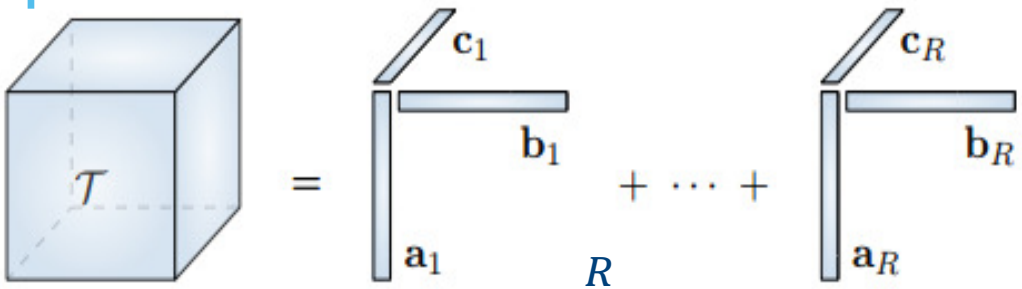
Nele Moelans; 6/03/2017


IX
III
VIII
IV
VII
V
VI
Line Microstructure
VIII/IX α+γ<γ>α+γ>β
IX/III α+γ<γ>β
III/IV α+γ<γ|β
IV/V α+γ<β
V/VI α+γ<α|β
VII/VIII α+γ|α+γ>α>β
Area Microstructure
I α+γ|α+γ>β
II α+γ|α+γ>γ>β
III α+γ<γ>β
IV α+γ<γ<β
V α+γ<α<β
VI α+γ<α>β
VII α+γ|α+γ>α>β
C
B
A
γ
α
β
X_C
X_B


Parameters
Simulations
Great challenge
Principle elements
2-3 elements
High entropy alloys

Tensor decomposition

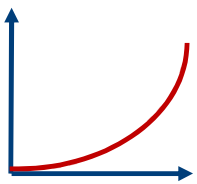
3D:

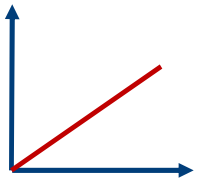


$$t_{ijk} = \sum_{r=1}^{R} a_{ir} b_{jr} c_{kr}$$

I^3 elements → $3*I*R$ data points

ND: I^N elements → $N*I*R$ data points





Thermodynamics Ag-Cu-Ni-Sn liquids

$$G(x_{Ag}, x_{Cu}, x_{Sn}, T) - G_{log} = \sum_{r=1}^{4} a_{ir} b_{jr} c_{kr} d_{lr}$$

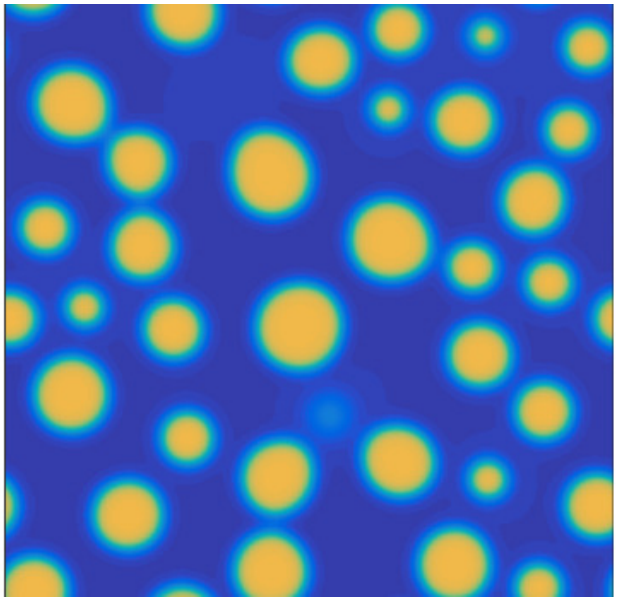
8 e12 elements

Error < 1%

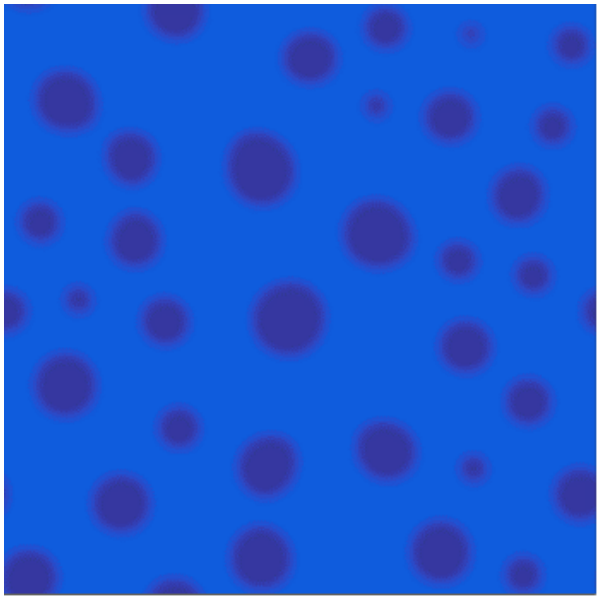
$$a = \left(\text{Ag}^{4} \right)^{10000}, \quad b = \left(\text{Cu}^{4} \right)^{10000}, \quad c = \left(\text{Ni}^{4} \right)^{10000}, \quad d = \left(T^{4} \right)^{\infty}$$

1,2 e5 data points

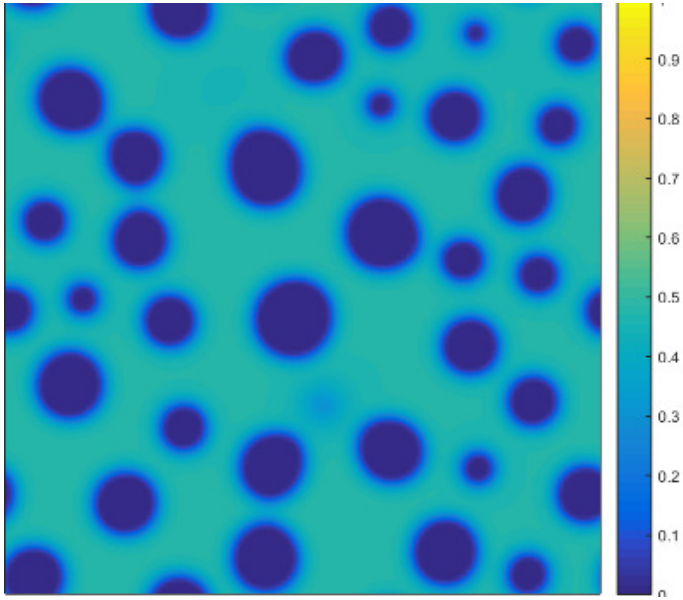
Phase-field model Ag-Cu-Ni-Sn liquid



$x_{Ag}(x, y, z, t')$



$x_{Cu}(x, y, z, t')$



$x_{Ni}(x, y, z, t')$

$$\frac{\partial x_{Ag}(x, y, t)}{\partial t} = \nabla M \cdot \nabla \left[\frac{\partial G\left(x_{Ag}, x_{Cu}, x_{Ni}, T\right)}{\partial x_{Ag}} - \varepsilon \nabla^2 x_{Ag} \right]$$

ERC-2016-StG INTERDIFFUSION

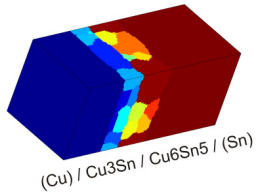
Nucleation/ elastoplastic models

DFT based approaches

Gibbs energy/ diffusion mobility models (CALPHAD)

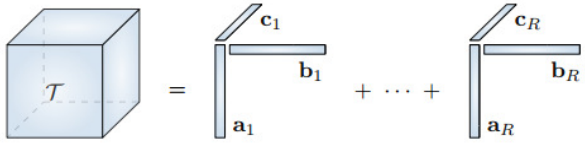
Innovative & high potential idea

Phase-field simulations



$$\frac{\partial \varphi}{\partial t} = -L\left[\frac{\partial G}{\partial \varphi} - \nabla^2 \varphi\right]$$

Tensor decomposition



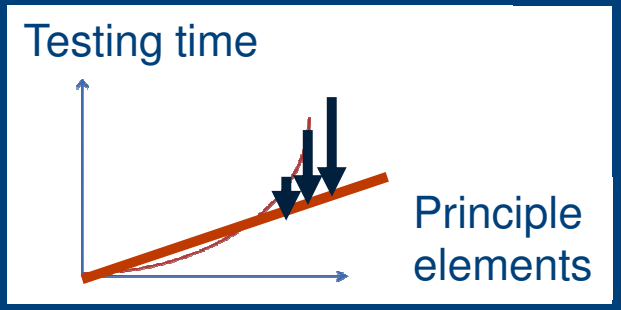
$I^N \rightarrow R*N*I$

Microstructure characteristics (comp, t, Temp, …)

Breakthroughs

- Simulations with 5-8 elements
- (Re)Interpretation experiments
- Search & Discovery

→ Accelerated material & product design



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	Implementation/ Validation module (month 1-24)	Discovery module (month 1-60)	Multi-material design module *(postdoc, month 25-60)*
Tensor decomposition			
(PhD 4, month 13-60)			

± 45500 simulations

130 variables (N), 50 values (I), assume R = 7

Corresponds to $50^{130} \approx 10^{220}$ tensor elements

Thank you !

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